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THE UNITED STATES PATENT AND TRADEMARK OFFICE

Applicants: Yuan-Ping Pang

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Serial No. : 09/595,650

Examiner : M. Sheinberg

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Title : MOLECULAR MODELING FOR METALLOPROTEINS

Assistant Commissioner for Patents  
Washington, D.C. 20231

**RESPONSE AND AMENDMENT**

This communication is responsive to the Office Action mailed August 16, 2001 (paper No. 8, hereafter referred to as "OA") and the telephonic interview held November 15, 2001. Applicant wishes to thank Examiner Sheinberg and Examiner Marshall for agreeing to conduct a telephonic interview. Applicant believes that agreement was reached during the telephonic interview concerning some of the Examiner's rejections. Applicant will note in the remarks section where Applicant believes that agreement was reached. Reconsideration of the claim rejections is respectfully requested in view of the following amendments and remarks.

**Amendments**

Please amend claims 37 to 54, and add claims 55 to 72 as follows:

37. (amended) A computer readable medium having data structures stored thereon, comprising a data structure to store a simulated metal ion for use in a molecular dynamics simulation comprising a center atom having a van der Waals radius greater than zero covalently linked to one or more dummy atoms having a van der Waals radius of about zero, wherein the overall charge of said metal ion is evenly

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55. (new) A computer readable medium having computer executable instructions stored thereon, that when executed simulate a metal ion for use in a molecular dynamics simulation comprising a center atom having a van der Waals radius greater than zero covalently linked to one or more dummy atoms having a van der Waals radius of about zero, wherein the overall charge of said metal ion is evenly distributed among said dummy atoms and wherein said center atom has a charge of zero.
56. (new) The computer readable medium of claim 55 wherein said dummy atom has a mass of about 0.1 g/mol.
57. (new) The computer readable medium of claim 55 wherein said dummy atom has a mass greater than about 0.1 g/mol.
58. (new) The computer readable medium of claim 55 wherein said dummy atoms are located at the apices of a polyhedron.
59. (new) The computer readable medium of claim 58 wherein said center atom is located at the center of said polyhedron.
60. (new) The computer readable medium of claim 58 wherein said polyhedron is selected from the group consisting of trigonal, tetrahedron, pentahedron, hexagonal, septagonal, and octahedral.
61. (new) The computer readable medium of claim 59 wherein said polyhedron is a tetrahedron.
62. (new) The computer readable medium of claim 55 wherein said metal ion is selected from a main group metal or transition metal.

63. (new) The computer readable medium of claim 55 wherein said metal ion is selected from the group consisting of zinc, cadmium, mercury, copper, nickel, cobalt, iron, manganese, calcium, and magnesium.
64. (new) The computer readable medium of claim 55 wherein said metal ion is zinc.
65. (new) The computer readable medium of claim 59 wherein said metal ion is zinc.
66. (new) The computer readable medium of claim 55 wherein said metal ion is magnesium.
67. (new) The computer readable medium of claim 55 wherein said metal ion is calcium.
68. (new) The computer readable medium of claim 55 wherein said metal ion has a calculated energy of solvation about equal to an experimentally determined energy of solvation for said metal ion.
69. (new) The computer readable medium of claim 68 wherein said calculated energy of solvation is within about 10% of said experimentally determined energy of solvation for said metal ion.
70. (new) The computer readable medium of claim 55 wherein said dummy atom has a charge of about 0.5.
71. (new) The computer readable medium of claim 55 wherein said dummy atom has a charge of about 0.3333.
72. (new) The computer readable medium of claim 55 wherein said dummy atom has a charge ranging from about +0.1 to about +3.